Cyclopropanecarboxylic acid, 1-((4-chlorophenyl)sulfonyl)-, 1-methylethyl ester

145348-23-8 | DTXSID20162992

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.70

Global applicability domain: Inside

Local applicability domain index: 6.17e-01

Confidence level: 8.10e-01

Nearest Neighbors from the Training Set

Image not found
Cyclopropanecarboxylic acid, 1-
((4-chlorophenyl)sulfonyl)-, 1-
methylethyl ester
Measured: 2.64
Predicted: 2.70

Image not found
Cyclopentanecarboxylic acid, 1-
((4-bromophenyl)sulfonyl)-,
methyl ester
Measured: 2.73
Predicted: 2.64

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Cyclobutanecarboxylic acid, 1-
((4-methylphenyl)sulfonyl)-, 1-
methylethyl ester
Measured: 2.78
Predicted: 2.50

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Cyclobutanecarboxylic acid, 1-
((4-bromophenyl)sulfonyl)-,
methyl ester
Measured: 2.45
Predicted: 2.49

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Cyclohexanecarboxylic acid, 1-
((4-bromophenyl)sulfonyl)-,
methyl ester
Measured: 2.94
Predicted: 2.84